

Convex politopes and quantum separability

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We advance a novel perspective of the entanglement issue that appeals to the Schlienz-Mahler measure [Phys. Rev. A **52**, 4396 (1995)]. Related to it, we propose a criterium based on the consideration of convex subsets of quantum states. This criterium generalizes a property of product states to convex subsets (of the set of quantum-states) that is able to uncover a new geometrical property of the separability property.

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I. INTRODUCTION

Schrödinger stated, as everyone knows, that “entanglement is **the** characteristic trait of quantum mechanics” [1–3]. Many years afterwards, entanglement, although still rather a puzzling issue, is a subject of immense attention, mostly because interest on its characterization has more than foundational significance, it being a powerful resource for quantum information processing that offers a host of possible technological applications [4]. A suggestive assertion [5, 6] seemingly deserves repetition: “The fundamental question in quantum entanglement theory is *which states are entangled and which are not*”.

A. Abstract mathematical notions and entanglement

The geometric properties of entanglement are of paramount importance (see [5]). In order to characterize it, many mathematical strategies have been followed, that range from the application of algebraic tools, to group theory, differential geometry, convex geometry, numerical simulations, etc. (see [5–7]). Without any doubt, the discovery of new mathematical structures underlying the theoretical description of entanglement has provided insightful answers to the problems of its characterization, manipulation and quantification, as remarked in [7]. Underlying many of these approaches, one encounters once and again geometrical properties of

the quantum set of states and, in particular, those of the set of separable states [8]. For examples of geometrical applications to the study of entanglement see, for instance, [10–19] and also [9] for an excellent overview.

Since characterizing the geometry of entanglement is indeed a fundamental task for physicists, *we propose here to appeal to a very powerful abstract concept for guiding entanglement-research, namely, the convex set of quantum states (CSQS)*, which exhibits fascinating geometrical properties [9]. The CSQS not only deserves mathematical interest, but also sheds light on the abstract and counterintuitive properties of entanglement, the difference between entangled and separable states being a conspicuous example [8]. In a different vein, information needed to reformulate quantum mechanics is fully contained in the geometrical properties of the quantum set of states [20–22]. Summing up: geometrical knowledge about these properties underlies most of the current research-lines on entanglement and opens the door to the possibility of exploring non-linear generalizations of quantum mechanics. See also [23–29] for more examples of geometrical applications. It seems odd to regard any piece of mathematics as too abstract for entanglement-physicists.

B. Our goal

This work pretends to exhibit *unexplored* geometrical properties of separable states and also present a novel separability criterium (SC) closely linked

to the Schlienz-Mahler (SM) entanglement measure [30]. Our SC is formulated in geometrical-convexity terms and is easily exportable to more general environments via the so-called convex operational approach to physics.

Now, the SM measure alluded to above constitutes a really significant development, being used as a basis not only for developing new ideas but also to establish separability criteria (see for example [31], [32], [33], [34], and [35]). Their authors (SM) focus attention *on the difference between a given density matrix and the product of its reduced states* $\rho^A \otimes \rho^B$. We will use a suitable generalization of this difference in order to establish a link between the convex sets of the compound system and its subsystems, thereby developing a new entanglement criterium based on the convex structure of the set of quantum states. A similar derivation can be made by recourse to a quantum logical approach [36]. Our admittedly abstract criterium can still shed some light on the geometrical properties of separable states.

In working with the convex structure of the quantum set of states we will regard convex subsets of it as probability spaces and take advantage of the fact that some of these subsets can be fully recovered from the information contained on the available states of the associated subsystems. Such is our leit motif. Further, we will advance the notion of informational invariance and deal with *convex invariant subsets*. Our proposal is based on the property that for every separable state there exists a convex subset which contains it and is an informational invariant. From such basic idea, our entanglement-edifice will be built up. It is endowed with the strength of possibly allowing one to study and classify entanglement in higher dimensions, and even to multipartite systems just because of its abstract nature.

Matters are organized as follows. After some preliminaries (which, though not essential for the rest of the article, may serve as a conceptual and mathematical guide) in Sec. II, we review in section III some ideas of [30] together with their consequences. In section IV we show how to construct special functions that allow us to develop a new separability criterium. In section V we discuss implications of this criterium and indicate how the functions so developed can be used to generalize product states to convex sets. In section VI we condense some of our results in a more conceptual fashion and, finally, draw some conclusions.

II. PRELIMINARIES

The mathematically savvy reader should skip this Section. Given a composite-system formed of subsystems A and B , a fundamental characteristic of a product state, i.e., a state of the form

$$\rho_{Prod} = \rho^A \otimes \rho^B \quad (1)$$

is that information of the whole state may be reconstructed from the simple sum of the information on the states of the subsystems. The “simple sum” is mathematically represented by taking tensor products on the reduced states of the subsystems. Thus the above statement may be expressed in mathematical terms: taking partial traces and making tensor products leave the state unchanged. But not every separable state has this property; in general, a separable state will be of a non-product kind, and the above informational relationship is no longer true. No entangled state has this property. Thus, only product states are *invariant* in this sense. Product states are fully recovered from the information contained in the states of the subsystems (to be abbreviated as the “reobtained” property). We may call this property the *informational invariance*.

We may also ask, and this is an unconventional viewpoint, for the subsets of the convex set of states that exhibit the recoverable property. An important example is the whole set of separable states itself. It has -by definition- the property of being fully recoverable by making tensor products of the complete set of states of the subsystems and closing them by mixing operation [8]. In this sense we recover the informational invariance property referred to above. Given the set of available states of two systems, a physical operation is that of taking tensor products and then mix the pertinent states. States obtained using these operations (together with local unitary evolutions and classical communication) are classically reproducible [8]. *In this work we give a precise mathematical formulation for set-notions of the kind exemplified above, as well as a geometrical characterization of them.* The ensuing mathematical notions will reveal novel geometrical structures which, in turn, make room for a better characterization of quantum states.

We will denote sets of states with the informational invariance property as *convex separable subsets* (CSS) and will show that for every separable state there exists a convex subset which contains it and is an informational invariant (strictly included in the convex set of separable states). Such indeed is the basis of our abstract separability criterium, to be advanced below. Another important feature of our abstract construction is the attainment of a

purely geometrical description based on the convex structure of the quantum set of states. The associated geometric reformulation of entanglement may be useful for generalizing it to more general scenarios, based on convex sets [39–41].

A. Basic math-definitions

We remind the reader that every subset A of a vector space is contained within a smallest convex set called the convex hull of A , namely the intersection of all convex sets containing A . Thus, it is possible to define a convex-hull map $\text{Conv}()$ which has three characteristic properties: i) extensivity $A \subseteq \text{Conv}(A)$, ii) non-decreasing nature $A \subseteq B$ implies that $\text{Conv}(A) \subseteq \text{Conv}(B)$, and iii) idempotency $\text{Conv}(\text{Conv}(A)) = \text{Conv}(A)$. Also, an extremal point of a convex set S in a real vector space is a point in S which does not lie in any open line segment joining two points of S (an extremal point would be a “corner” of S). An important example for quantum mechanics is that of pure states: they are the extreme points of the CSQS (more on this below).

A convex polytope may be defined as the convex hull of a finite set of points (which are always bounded), or as a bounded intersection of a finite set of half-spaces. One often asserts that the term “polytope” is i) the general vocable of the sequence “point, line segment, polygon, polyhedron, ...,” or ii) to be regarded as a finite region of an n -dimensional space enclosed by a finite number of hyperplanes. A d -dimensional polytope may be specified as the set of solutions to a system of linear inequalities

$$M\mathbf{x} \leq \mathbf{b}, \quad (2)$$

where M is a real $s \times d$ matrix, and \mathbf{b} is a real s -vector.

For quantum systems, $\mathcal{P}(\mathcal{H})$ will denote the set of all closed subspaces of the pertinent Hilbert space \mathcal{H} , which are in a one to one correspondence with the projection operators. Because of this one to one link, one usually employs the notions of “closed subspace” and “projector” in interchangeable fashion. An important construct is \mathcal{A} , the set of bounded Hermitian operators on \mathcal{H} , while the bounded operators on \mathcal{H} will be denoted by $\mathcal{B}(\mathcal{H})$. Pure quantum states may be put in correspondence with the projective space $\mathbf{CP}(\mathcal{H})$ of a complex Hilbert space \mathcal{H} , which is the set of equivalence classes of vectors v in \mathcal{H} , with $v \neq 0$, for the

relation given by $v \sim w$ when $v = \lambda w$ with λ a non-zero scalar. Here the equivalence classes for \sim are also called projective rays. A trace class operator is a compact one for which a finite trace may be defined (independently of the choice of basis).

We will appeal below to the set \mathcal{C} containing all positive, hermitian, and trace-class (normalized to unity) operators in $\mathcal{B}(\mathcal{H})$. *A larger and important structure used below, is the one denoted by $\mathcal{L}_{\mathcal{C}}$, the set of all convex subsets of \mathcal{C} .* This structure is endowed with a lattice structure. Finally, the reader may wish to recall in the Appendix some elementary set-theory concepts used in the text. It is important to remark that we will restrict to the finite dimensional case in the rest of this work.

III. THE SCHLIENZ-MAHLER ENTANGLEMENT MEASURE

For two quantum systems S_1 and S_2 , if $\{|\varphi_i^{(1)}\rangle\} - \{|\varphi_i^{(2)}\rangle\}$ are the corresponding orthonormal basis of $\mathcal{H}_1 - \mathcal{H}_2$, respectively, then the set $\{|\varphi_i^{(1)}\rangle \otimes |\varphi_j^{(2)}\rangle\}$ constitutes an orthonormal basis for $\mathcal{H}_1 \otimes \mathcal{H}_2$. A general (pure) state of the composite $S_1 - S_2$ system can be written as:

$$\rho = |\psi\rangle\langle\psi|. \quad (3)$$

with $|\psi\rangle$ any vector in $\mathcal{H}_1 \otimes \mathcal{H}_2$. In the finite dimensional case mixtures are represented by positive, Hermitian and trace one operators (also called ‘density matrices’). The set of all density matrixes forms a convex set (of states), which was called \mathcal{C} above, while the physical observables are represented by elements of \mathcal{A} , the vector space of Hermitian operators acting on \mathcal{H} . Formally we deal with the sets

Definition III.1. $\mathcal{A} := \{A \in \mathcal{B}(\mathcal{H}) \mid A = A^\dagger\}$

Definition III.2. $\mathcal{C} := \{\rho \in \mathcal{A} \mid \text{tr}(\rho) = 1, \rho \geq 0\}$,

where $\mathcal{B}(\mathcal{H})$ stands for the algebra of bounded operators in \mathcal{H} . \mathcal{C} is a convex set inside the hyperplane $\{\rho \in \mathcal{A} \mid \text{tr}(\rho) = 1\}$ formed by the intersection of this hyperplane with the cone of positive matrices (see Figure 1). Separable states are defined [8, 9] as those states of \mathcal{C} which can be written as a convex combination of product states:

$$\rho_{\text{Sep}} = \sum_{i,j} \lambda_{ij} \rho_i^{(1)} \otimes \rho_j^{(2)}, \quad (4)$$

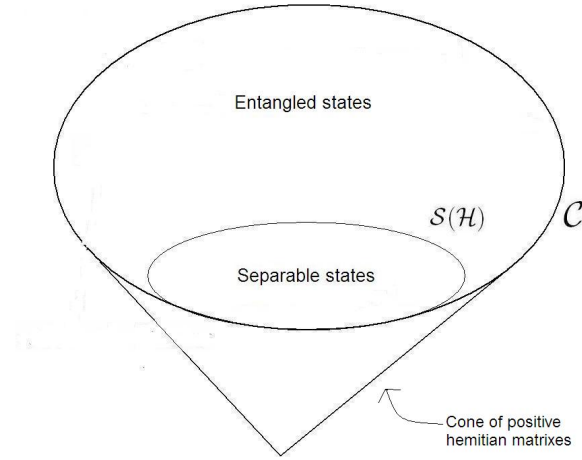


FIG. 1. Geometric representation of the convex set of states.

where $\rho_i^{(1)} \in \mathcal{C}_1$, and $\rho_j^{(2)} \in \mathcal{C}_2$, $\sum_{i,j} \lambda_{ij} = 1$ and $\lambda_{ij} \geq 0$. We denote the set of separable states by $\mathcal{S}(\mathcal{H})$.

In set-parlance, the collective of entangled states becomes precisely defined by

$$\mathcal{E}(\mathcal{H}) := \mathcal{C} \setminus \mathcal{S}(\mathcal{H}), \quad (5)$$

where “ \setminus ” stands for set-theoretical difference.

As the dimension of the Hilbert space grows, most

of the states in \mathcal{C} are non separable [37]. The estimation of the volume of $\mathcal{S}(\mathcal{H})$ is of great interest (see –among others– [27], [37] and [38]). The entanglement measure advanced in [30] is based on the Fano decomposition [42] (see also [9], page 349). For $\rho \in \mathcal{C}$, if the dimension of the Hilbert space is d , one expresses it in terms of $\{\sigma_i\}$, the $d^2 - 1$ generators of $SU(d)$ (the group of special unitary matrixes acting on \mathcal{H}). For composite bipartite systems, if $d = NK$, then we have the following decomposition (in terms of the basis $SU(N) \otimes SU(K)$)

$$\rho = \frac{1}{NK} (\mathbf{1}_{NK} + \sum_{i=1}^{N^2-1} \tau_i^A \sigma_i \otimes \mathbf{1}_K + \sum_{j=1}^{K^2-1} \tau_j^B \mathbf{1}_N \otimes \sigma_j + \sum_{i=1}^{N^2-1} \sum_{j=1}^{K^2-1} \beta_{ij} \sigma_i \otimes \sigma_j), \quad (6)$$

where τ_i^A and τ_j^B are Bloch vectors such that

$$\rho^A = \frac{1}{N} (\mathbf{1}_N + \sum_{i=1}^{N^2-1} \tau_i^A \sigma_i), \quad (7)$$

with an analogous form for ρ^B . ρ^A and ρ^B are the reduced density matrixes of subsystems A and B respectively. Schlienz-Mahler (SM) note that the term $\sum_{i=1}^{N^2-1} \sum_{j=1}^{K^2-1} \beta_{ij} \sigma_i \otimes \sigma_j$ is related to corre-

lations and proceed to construct an entanglement measure using it. SM define then the tensor

$$M_{ij} = \beta_{ij} - \tau_i^A \tau_j^B, \quad (8)$$

that will play a leading role in their considerations. They use $\text{tr}(\mathbf{M}\mathbf{M}^\dagger)$ as a measure of entanglement (up to normalization), and this measure conveys essentially the same information as

$$\|\rho - \rho^A \otimes \rho^B\|_{\mathcal{HS}}^2, \quad (9)$$

where $\|\cdots\|_{\mathcal{HS}}$ is the Hilbert Schmidt norm

$$\|A\|_{\mathcal{HS}}^2 = \text{tr}(AA^\dagger), \quad (10)$$

for any $A \in \mathcal{B}(\mathcal{H})$. The measure (9)

- vanishes for any product state,
- is positive elsewhere,
- it is maximal for any pure state with vanishing Bloch vectors τ_i^A and τ_j^B (Equation (7)), and
- it is invariant under local unitary transformations.

Such properties allow for the development of other entanglement measures and entanglement criteria (see, for example, [35]). The distance induced by the trace norm between two states represents how well two states can be distinguished via measurement [43]. It can be shown [34] that

$$\sum_{i,j=1}^3 C^2(\hat{\sigma}_i^A, \hat{\sigma}_j^B) = 4\text{tr}[(\rho - \rho^A \otimes \rho^B)^2], \quad (11)$$

with

$$C(\sigma_i^A, \sigma_j^B) = \langle \sigma_i^A \otimes \sigma_j^B \rangle - \langle \sigma_i^A \otimes \mathbf{1}^B \rangle \langle \mathbf{1}^A \otimes \sigma_j^B \rangle, \quad (12)$$

making (9) easy to implement because it can be measured via single-rates and coincidence-rates. More generally, functions of the form

$$W(\rho) = \|F(\rho - \rho^A \otimes \rho^B)\|, \quad (13)$$

have been studied in some detail (see for example [32],[33], [34] and [35]). $\|\cdots\|$ denotes a norm on the space of density matrixes and $F : \mathcal{C} \rightarrow \mathcal{C}$ a useful function for the study of entanglement. Thus, entanglement measures (9) become special cases of (13). The conditions imposed on F and $\|\cdots\|$ are such that W satisfies a similar set of conditions than the ones imposed on the SM measure listed above.

In the following section we show that entanglement measures of the form (13) are closely linked to a particular separability criterium that generalizes the map which assigns $\rho^A \otimes \rho^B$ to any composite density matrix ρ .

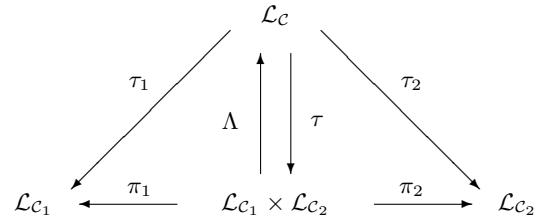


FIG. 2. The different maps between \mathcal{L}_{C_1} , \mathcal{L}_{C_2} , $\mathcal{L}_{C_1} \times \mathcal{L}_{C_2}$, and \mathcal{L}_C . π_1 and π_2 represent canonical projections.

IV. A NEW SEPARABILITY CRITERIUM

A. Preliminary matters

A glance at the Appendix might be useful at this stage. In the previous section we saw how to construct a family of entanglement measures via the mapping

Definition IV.1.

$$\Omega : \mathcal{C} \rightarrow \mathcal{C}$$

$$\rho \mapsto \rho^A \otimes \rho^B.$$

Product states $\rho = \rho^A \otimes \rho^B$ satisfy

$$\Omega(\rho^A \otimes \rho^B) = \rho^A \otimes \rho^B, \quad (14)$$

and they are the only states which satisfy (14). Our leading idea now is that of *generalizing the above considerations to convex subsets of \mathcal{C}* .

1. First notion-generalization

In order to do so let us first study maps onto the set of states of the subsystems, \mathcal{C}_1 and \mathcal{C}_2 . We start by defining special “mappings” using partial traces

$$\begin{aligned} \text{tr}_i : \mathcal{C} &\rightarrow \mathcal{C}_j \\ \rho &\mapsto \text{tr}_i(\rho), \end{aligned} \quad (15)$$

from which we can construct the induced maps τ_i on \mathcal{L}_C , the set of all convex subsets of \mathcal{C} (a similar definition for \mathcal{L}_{C_i} , $i = 1, 2$), via the image of any subset $C \subseteq \mathcal{C}$ under tr_i

$$\begin{aligned} \tau_i : \mathcal{L}_C &\rightarrow \mathcal{L}_{C_i} \\ C &\mapsto \text{tr}_j(C), \end{aligned} \quad (16)$$

where for $i = 1$ we take the partial trace with $j = 2$ and vice versa. Thus, we can define the product map

$$\begin{aligned}\tau : \mathcal{L}_C &\longrightarrow \mathcal{L}_{C_1} \times \mathcal{L}_{C_2} \\ C &\mapsto (\tau_1(C), \tau_2(C))\end{aligned}\quad (17)$$

which generalizes partial traces to convex subsets of \mathcal{C} .

In order to complete the desired generalization, let us now define for convex subsets a new set-operation $C_1 \otimes C_2$ that might be regarded as the analogous of the tensor product (see Figure 2). We are thus, loosely speaking, dealing with “quasi-tensor set-compositions” and accordingly introduce the set of the definition that follows:

Definition IV.2. *Given convex subsets $C_1 \subseteq \mathcal{C}_1$ and $C_2 \subseteq \mathcal{C}_2$ we consider the set constructed according to*

$$C_1 \tilde{\otimes} C_2 := \{\rho_1 \otimes \rho_2 \mid \rho_1 \in C_1, \rho_2 \in C_2\} \quad (18)$$

The symbol “ $\tilde{\otimes}$ ” has a tilde in order to avoid confusing it with the usual product of convex sets. Using this, we define the map:

Definition IV.3.

$$\Lambda : \mathcal{L}_{C_1} \times \mathcal{L}_{C_2} \longrightarrow \mathcal{L}_C$$

$$(C_1, C_2) \mapsto \text{Conv}(C_1 \otimes C_2)$$

where $\text{Conv}(\dots)$ stands for *convex hull* of a given set. Applying Λ to the particular case of the quantum sets of states of the subsystems (C_1 and C_2), one sees that Definitions IV.2 and IV.3 entail

$$\Lambda(C_1, C_2) = \text{Conv}(C_1 \tilde{\otimes} C_2) \quad (19)$$

and so, this is nothing but

$$\Lambda(C_1, C_2) = \mathcal{S}(\mathcal{H}) \quad (20)$$

because $\mathcal{S}(\mathcal{H})$ is by definition (for finite dimension) the convex hull of the set of all product states (which equals to $C_1 \tilde{\otimes} C_2$). Thus, the map Λ gives a precise mathematical expression for the operation of making tensor products and mixing mentioned in Section II. Additionally, if $\rho = \rho_1 \otimes \rho_2$, with $\rho_1 \in C_1$ and $\rho_2 \in C_2$, then $\{\rho\} = \Lambda(\{\rho_1\}, \{\rho_2\})$, with $\{\rho_1\} \in \mathcal{L}_{C_1}$, $\{\rho_2\} \in \mathcal{L}_{C_2}$ and $\{\rho\} \in \mathcal{L}_C$. We can demonstrate as well that

Proposition IV.4. *Let $\rho \in \mathcal{S}(\mathcal{H})$. Then, there exist $C \in \mathcal{L}_C$, $C_1 \in \mathcal{L}_{C_1}$, and $C_2 \in \mathcal{L}_{C_2}$ such that $\rho \in C = \Lambda(C_1, C_2)$.*

Proof. If $\rho \in \mathcal{S}(\mathcal{H})$, then $\rho = \sum_{ij} \lambda_{ij} \rho_i^1 \otimes \rho_j^2$, with $\sum_{ij} \lambda_{ij} = 1$ and $\lambda_{ij} \geq 0$. Consider now the convex sets

$$\begin{aligned}C_1 &= \text{Conv}(\{\rho_1^1, \rho_2^1, \dots, \rho_k^1\}) \\ C_2 &= \text{Conv}(\{\rho_1^2, \rho_2^2, \dots, \rho_l^2\}).\end{aligned}\quad (21)$$

We define:

$$C := \Lambda(C_1, C_2) = \text{Conv}(C_1 \otimes C_2). \quad (22)$$

Clearly, the set $\{\rho_i^1 \otimes \rho_j^2\} \subseteq C_1 \otimes C_2$, and then $\rho \in C$. \square

2. Second notion-generalization

The next notion to be tackled needs perhaps a perusal of section II.A. We pass now to the generalization to convex subsets of the map Ω in Definition IV.1. This is the function $\Lambda \circ \tau$ (the composition of τ with Λ). For the special case of a convex set formed by only one “matrix” (point) $\{\rho\}$ we have

$$\Lambda \circ \tau(\{\rho\}) = \{\rho^A \otimes \rho^B\} \quad (23)$$

which is completely equivalent to Ω and thus satisfies (14). In what follows we will need a proposition taken from [44]. It reads:

Proposition IV.5. *Let S be a subset of a linear space \mathcal{L} . Then $x \in \text{Conv}(S)$ iff x is contained in a finite dimensional polytope Δ whose extremal points belong to S ,*

This is all we need to formulate now our proposal in the next subsection.

B. Our separability proposal

We will here “traduce” the idea of non separability as a special kind of set-theory relationship.

Proposition IV.6. *If ρ is a separable state, then there exists a convex set (indeed, a polytope), $S_\rho \subseteq \mathcal{S}(\mathcal{H})$ such that $\rho \in S_\rho$ and $\Lambda \circ \tau(S_\rho) = S_\rho$. More generally, for a convex set $C \subseteq \mathcal{S}(\mathcal{H})$, there exists a convex set $S_C \subseteq \mathcal{S}(\mathcal{H})$ such that $\Lambda \circ \tau(S_C) = S_C$. For a product state, we can choose $S_\rho = \{\rho\}$. For any convex set $C \subseteq \mathcal{C}$ which has at least one non-separable state it is true that there is no convex set S such that $C \subseteq S$ and $\Lambda \circ \tau(S) = S$.*

Proof. We have already seen above that if ρ is a product state, then $\Lambda \circ \tau(\{\rho\}) = \{\rho\}$ and thus $S_\rho = \{\rho\}$. If ρ is a general separable state, then there exists $\rho_k^1 \in \mathcal{C}_1$, $\rho_k^2 \in \mathcal{C}_2$ and $\alpha_k \geq 0$, $\sum_{k=1}^N \alpha_k = 1$ such that $\rho = \sum_{k=1}^N \alpha_k \rho_k^1 \otimes \rho_k^2$. Now consider the convex set (a polytope)

$$M = \left\{ \sigma \in \mathcal{C} \mid \sigma = \sum_{i,j=1}^N \lambda_{ij} \rho_i^1 \otimes \rho_j^2, \right. \\ \left. \lambda_{ij} \geq 0, \sum_{i,j=1}^N \lambda_{ij} = 1 \right\} \quad (24)$$

M contains all convex combinations of products of

the elements which appear in the decomposition of ρ . It should be clear that $\rho \in M$. Let us compute $\Lambda \circ \tau(M)$, with $\tau(M) = (\tau_1(M); \tau_2(M))$. An element of $\tau_1(M)$ is of the form (for $\sigma \in M$)

$$\text{tr}_1(\sigma) = \sum_{i=1}^N \left(\sum_{j=1}^N \lambda_{ij} \right) \rho_i^1 = \sum_{i=1}^N \mu_i \rho_i^1, \quad (25)$$

with $\mu_i = \sum_{j=1}^N \lambda_{ij}$. In analogous fashion we show that an element of $\tau_2(M)$ is of the form $\sum_{j=1}^N \nu_j \rho_j^2$ with $\nu_i = \sum_{i=1}^N \lambda_{i,j}$. Note that $\sum_{j=1}^N \mu_j = \sum_{j=1}^N \nu_j = 1$. In order to compute $\Lambda(\tau_1(M); \tau_2(M))$ we must build the convex hull of the set

$$\tau_1(M) \widetilde{\otimes} \tau_2(M) = \{ \sigma_1 \otimes \sigma_2 \mid \sigma_1 \in \tau_1(M), \sigma_2 \in \tau_2(M) \} = \left\{ \sum_{i,j=1}^N \mu_i \nu_j \rho_i^1 \otimes \rho_j^2 \right\}. \quad (26)$$

and we conclude that

$$\Lambda \circ \tau(M) = \text{Conv} \left(\left\{ \sum_{i,j=1}^N \mu_i \nu_j \rho_i^1 \otimes \rho_j^2 \right\} \right). \quad (27)$$

Let us prove that $\Lambda \circ \tau(M) = M$. If $\sigma \in \Lambda \circ \tau(M)$, by looking at equation (27) it is apparent that σ belongs to M . On the other hand, if $\sigma \in M$, then $\sigma = \sum_{i,j=1}^N \lambda_{i,j} \rho_i^1 \otimes \rho_j^2$ (convex combination). Note that $\Lambda \circ \tau(M)$ is a convex set because trace operators preserve convexity and Λ is a convex hull. On the other hand, $\Lambda \circ \tau(\{\rho_i^1 \otimes \rho_j^2\}) = \{\rho_i^1 \otimes \rho_j^2\}$, and, via the definition of $\tau_1(M) \widetilde{\otimes} \tau_2(M)$, we have that $\{\rho_i^1 \otimes \rho_j^2\} \in \Lambda \circ \tau(M)$ for all i, j . Thus, by the convexity of $\Lambda \circ \tau(M)$, $\sigma \in \Lambda \circ \tau(M)$, which concludes the proof that $\Lambda \circ \tau(M) = M$ (and that M is a polytope). Consequently, M is the desired $S_\rho \subseteq \mathcal{S}(\mathcal{H})$.

If a given subset $C \subseteq \mathcal{S}(\mathcal{H})$ then all $\rho \in C$ are separable. $\mathcal{S}(\mathcal{H})$ is, by definition, a convex set. Let us see that it is invariant under $\Lambda \circ \tau$. First of all, we know that $\mathcal{S}(\mathcal{H})$ is formed by all possible convex

combinations of products of the form $\rho_1 \otimes \rho_2$, with $\rho_1 \in \mathcal{C}_1$ and $\rho_2 \in \mathcal{C}_2$. But for each one of these tensor products, $\Lambda \circ \tau(\{\rho_1 \otimes \rho_2\}) = \{\rho_1 \otimes \rho_2\}$, and it is easy to see that they belong to $\Lambda \circ \tau(\mathcal{S}(\mathcal{H}))$. Since this is a convex set, all its convex combinations belong to it. Thus, we conclude that

$$\Lambda \circ \tau(\mathcal{S}(\mathcal{H})) = \mathcal{S}(\mathcal{H}). \quad (28)$$

This shows that for every $C \subseteq \mathcal{S}(\mathcal{H})$ we can find an invariant convex subset which is $\mathcal{S}(\mathcal{H})$ itself.

Note here that there are cases in which the set $C \subseteq \mathcal{S}(\mathcal{H})$ may be a proper subset (this is the case, for example, of product states) or a polytope when we consider separable but non-product states. We remember at this point the structural concept described by a definition of section II.A. Consider $C \in \mathcal{L}_C$ such that there exists a given $\rho \in C$ with ρ *nonseparable*. Now, $\Lambda \circ \tau(S) \subseteq \mathcal{S}(\mathcal{H})$ for all $S \in \mathcal{L}_C$. Then, it could never happen that there exists $S \in \mathcal{L}_C$ such that $C \subseteq S$ and $\Lambda \circ \tau(S) = S$. \square

From the last proposition we derive our separability criterium in terms of properties of convex sets that are polytopes:

Proposition IV.7. $\rho \in \mathcal{S}(\mathcal{H})$ if and only if there exists a polytope S_ρ such that $\rho \in S_\rho$ and $\Lambda \circ \tau(S_\rho) = S_\rho$.

In Figure 3 we display a geometric representation of the polytope S_ρ for a separable state. We see that the function $\Lambda \circ \tau$ is sensible to entanglement if applied to convex subsets of \mathcal{C} . Looking at (23),

it is also clear that $\Lambda \circ \tau$ is a generalization of Ω to convex subsets of \mathcal{C} .

With this extension, Proposition VI.1 asserts that

A state is separable if and only if it belongs to an invariant polytope of $\Lambda \circ \tau$. Separability entails membership in a special kind of convex set.

Clearly, starting from Proposition VI.1 we can derive the family of functions of the form (13). Why? Because if we restrict the function $\Lambda \circ \tau$ to convex sets formed by only one density matrix we obtain Equation (23) entailing that, if one knows that $\Lambda \circ \tau$ is sensible to entanglement via Proposition VI.1, it is natural to regard the norm of the difference between ρ and $\rho^A \otimes \rho^B$ as an entanglement measure's candidate. Our set-theory approach becomes then an *a posteriori* argument that in a sense “explains” the MS measure.

Let it be understood that we are restricting $\Lambda \circ \tau$ to one-element sets $\{\rho\}$. With some abuse of notation (which consists in avoiding the use of the kernels $\{\dots\}$) we write

$$\Lambda \circ \tau(\rho) := \rho^A \otimes \rho^B = \Omega(\rho) \quad (29)$$

V. GENERALIZED PRODUCT STATES

We delve here into an interesting analogy. Denote the set of product states by $\mathcal{S}_0(\mathcal{H})$. Restricting (29) to product states we have

$$\rho \in \mathcal{S}_0(\mathcal{H}) \Leftrightarrow \Lambda \circ \tau(\rho) = \rho \quad (\Leftrightarrow \Omega(\rho) = \rho) \quad (30)$$

From the discussion of the last section it is clear that our criterium is analogous to (30), being a generalization of it to convex subsets of \mathcal{C} because we have

$$\rho \in \mathcal{S}(\mathcal{H}) \Leftrightarrow \Lambda \circ \tau(S_\rho) = S_\rho, \quad (31)$$

with $\rho \in S_\rho$. Accordingly, we are in some sense generalizing a property of product states to any arbitrary separable state. As $\Lambda \circ \tau$ generally transforms any convex set into a different convex subset of $\mathcal{S}(\mathcal{H})$, (31) constitutes a geometrical property, characteristic of separable states. Thus, we advance here a “convex set” generalization of the notion of product state.

Definition V.1. A convex subset $C \subseteq \mathcal{C}$ such that $\Lambda \circ \tau(C) = C$ is called a convex separable subset (CSS) of \mathcal{C} .

Due to the arguments given above, product states are limit cases of convex separable subsets (they constitute the special case when the CSS has only one point).

An interesting open problem would then be that of looking for convex separable subsets of the function $\Lambda \circ \tau$. Looking at (28), we find that $\mathcal{S}(\mathcal{H})$ is a CSS (and indeed, the largest one). In this sense, CSS may be considered as small “copies” of $\mathcal{S}(\mathcal{H})$.

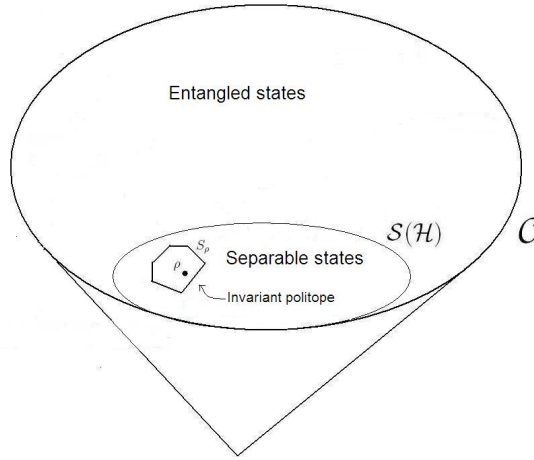


FIG. 3. Geometric representation of the invariant polytope which satisfies $\Lambda \circ \tau(S_\rho) = S_\rho$ and $\rho \in S_\rho$. ρ is separable if and only if there exists such a polytope.

In general, convex subsets of \mathcal{C} may be considered as probability spaces by themselves, because they are closed under convex combination of states. Thus, *CSS are probability spaces inside $\mathcal{S}(\mathcal{H})$* which are left invariant under the action of $\Lambda \circ \tau$ (and so, they have the same invariance property). The fact that $\mathcal{S}(\mathcal{H})$ is a CSS also tells us that the convex separable subsets can be more general sets and not necessarily just polytopes (because $\mathcal{S}(\mathcal{H})$ is not a polytope). Indeed, we may ask for ways to characterize the set of all convex separable subsets (which we denote by $\mathfrak{T}(\mathcal{C})$) by looking at the following property of Ω . If ρ is an arbitrary density matrix, then

$$\begin{aligned} \Omega^2(\rho) &= \Omega(\Omega(\rho)) = \Omega(\rho^A \otimes \rho^B) = \\ &\rho^A \otimes \rho^B = \Omega(\rho) \end{aligned} \quad (32)$$

or, in other words,

$$\Omega^2 = \Omega. \quad (33)$$

For $\Lambda \circ \tau$ and an arbitrary convex subset C one has

$$\begin{aligned} \Lambda \circ \tau(C) &= \Lambda(\tau_1(C), \tau_2(C)) = \\ &Conv(\tau_1(C) \tilde{\otimes} \tau_2(C)) \end{aligned} \quad (34)$$

If we apply $\Lambda \circ \tau$ again, we will find (with arguments expounded in the preceding section, see IV.6) that

$Conv(\tau_1(C) \tilde{\otimes} \tau_2(C))$ is a CSS. This, in turn, entails that

$$(\Lambda \circ \tau)^2 = \Lambda \circ \tau. \quad (35)$$

Consequently, our generalization of Ω satisfies an equality equivalent to (33). This fact can be gainfully used to characterize $\mathfrak{T}(\mathcal{C})$ as

$$\mathfrak{T}(\mathcal{C}) = \{\Lambda \circ \tau(C) \mid C \subseteq \mathcal{C}\}, \quad (36)$$

because, if C is a CSS, it is equal to $\Lambda \circ \tau(C)$, and thus we face one inclusion. The other inclusion comes from the fact that, for an arbitrary $C \subseteq \mathcal{C}$, (35) implies that $\Lambda \circ \tau(C)$ belongs to $\mathfrak{T}(\mathcal{C})$. Equation 36 simply asserts that $\mathfrak{T}(\mathcal{C})$ equals the image of $\mathcal{L}_\mathcal{C}$ under $\Lambda \circ \tau$.

Now we see that while in equation (13), the “core” was the function $\rho - \Lambda \circ \tau(\rho)$, now we have a new core

$$\Lambda \circ \tau(C) \setminus C, \quad (37)$$

where “ \setminus ” stands for set-theoretical difference, and we can try to measure the difference between C and its variation under $\Lambda \circ \tau$ in different ways. We will have a CSS if C and $\Lambda \circ \tau(C)$ coincide.

A possibility for measuring how different are C and $\Lambda \circ \tau(C)$ would entail looking for a generalization

of, for example, the relative entropy, which for a density matrix reads

$$S(\rho\|\sigma) = -\text{tr}(\rho \log(\sigma)) - S(\rho), \quad (38)$$

where $S(\rho) := -\text{tr}(\rho \log(\rho))$. Remark that the relative entropy concept has been used as a unifying approach for quantum and classical correlations [45]. When applied to convex subsets C and C' of \mathcal{C} , we are now conjecturing that

$$S(C\|C') := \inf_{\rho \in C, \sigma \in C'} S(\rho\|\sigma), \quad (39)$$

and use this conjecture to define

$$\tilde{F}(C) := S(\Lambda \circ \tau(C)\|C). \quad (40)$$

$\tilde{F}(C)$ clearly vanishes when $\Lambda \circ \tau(C) = C$, and in general, when $\Lambda \circ \tau(C) \cap C \neq \emptyset$. This last condition implies (in particular) that there are separable states which belong to C . We are free to use any divergence (or distance) instead of the relative entropy for the purpose of measuring the difference between C and $\Lambda \circ \tau(C)$ by making a similar construction.

Let us now study the segment joining ρ and $\Lambda \circ \tau(\rho)$. This segment is given by

$$L_\rho = \{x\rho + (1-x)\Lambda \circ \tau(\rho) \mid x \in [0, 1]\}. \quad (41)$$

If ρ is separable, using i) the polytope $S_\rho \subseteq \mathcal{S}(\mathcal{H})$ of proposition IV.6, ii) that ρ and $\Lambda \circ \tau(\rho)$ belong to S_ρ , and iii) that S_ρ is convex, we have

Proposition V.2.

$L_\rho \subseteq S_\rho \subseteq \mathcal{S}(\mathcal{H})$.

Coming back again to the demonstration of Proposition IV.6, and considering that the decomposition of a separable state as a convex combination of product states is not unique, we conclude that the invariant polytope is not unique. However, from the above proposition it is obvious that

$$L_\rho \subseteq \{\rho \in \mathcal{C} \mid \Lambda \circ \tau(C) = C \text{ and } \rho \in C\} \quad (42)$$

If there exists at least one nonseparable state in the segment joining ρ and $\Lambda \circ \tau(\rho)$, then ρ cannot be a separable state. This is a consequence of the convexity of $\mathcal{S}(\mathcal{H})$, but also follows from (42). Is

this fact of advantage for deciding on the separability of a given state? Indeed it is, if we use it in the following way. Given ρ , we parameterize the line segment between ρ and $\rho^A \otimes \rho^B$ as in proposition V.2. Afterwards, we apply this to all the points in the segment. If one finds a nonseparable state in the segment we conclude that ρ is nonseparable.

We consider now the action of the group of unitary local transformations of the form $U = U^1 \otimes U^2$ on the invariant polytope, where $U^{1,2} \in U^{\mathcal{K}^{1,2}}$. If $\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B$ is a separable state, then this action will be given by

$$U\rho U^\dagger = \sum_i p_i U^1 \rho_i^A U^{1\dagger} \otimes U^2 \rho_i^B U^{2\dagger}. \quad (43)$$

We can prove that

Proposition V.3. *If $\rho \in \mathcal{S}(\mathcal{H})$ and P_ρ is an invariant polytope (as the one in the demonstration of proposition IV.6), then $UP_\rho U^\dagger$ is an invariant polytope for $U\rho U^\dagger$.*

Proof. If $\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B$, then an invariant polytope is given by

$$P_\rho = \left\{ \sum_{i,j} \lambda_{ij} \rho_i^A \otimes \rho_j^B \mid \sum_{i,j} \lambda_{ij} = 1, \lambda_{ij} \geq 0 \right\}. \quad (44)$$

Because of the linearity of U , it is easy to see that P_ρ is transformed into

$$UP_\rho U^\dagger = \left\{ \sum_{i,j} \lambda_{ij} U^1 \rho_i^A U^{1\dagger} \otimes U^2 \rho_j^B U^{2\dagger} \mid \sum_{i,j} \lambda_{ij} = 1, \lambda_{ij} \geq 0 \right\}, \quad (45)$$

and as ρ is transformed as equation (43), then $UP_\rho U^\dagger$ is an invariant polytope. \square

The last proposition shows how invariant polytopes are transformed under unitary local transformations. As $\mathcal{S}(\mathcal{H})$ is invariant under these transformations, we see that they transform invariant polytopes into other invariant polytopes. Notice that V.3 implies (for invariant polytopes) that under an arbitrary local transformation U

$$\Lambda \circ \tau(UP_\rho U^\dagger) = UP_\rho U^\dagger = U(\Lambda \circ \tau(P_\rho))U^\dagger, \quad (46)$$

which reveals an interesting symmetry property of $\Lambda \circ \tau$.

VI. DISCUSSION

A. A conceptual analogy

For clarity's sake we condense here in a more conceptual fashion some of the technical implications of the foregoing sections via appeal to a comparison with the separability-notion for pure states. Its characterization in the bipartite is simple. $\rho = |\psi\rangle\langle\psi|$ will be separable if and only if it is a product of pure reduced states, i.e., if and only if there exist $|\phi_1\rangle \in \mathcal{H}_1$ and $|\phi_2\rangle \in \mathcal{H}_2$ such that $|\psi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle$. In mathematical terms (take care of not to be confused by equation (30))

$$|\psi\rangle\langle\psi| \in \mathcal{S}(\mathcal{H}) \Leftrightarrow \Lambda \circ \tau(|\psi\rangle\langle\psi|) = |\psi\rangle\langle\psi| \\ (\Leftrightarrow \Omega(|\psi\rangle\langle\psi|) = |\psi\rangle\langle\psi|). \quad (47)$$

It is well known that the case of mixed states is much more complicated than that of pure ones. But we may still ask if it is possible to develop a similar line of reasoning for mixed states. The existence of such a construction would allow for a more transparent view of the entanglement of mixed states (and thus for *all* states, generalizing (47)). The results and constructions presented in previous sections of this article indicate that a structure similar to that of equation (47) can indeed be constructed.

This fact makes for a remarkable analogy, unknown in the literature, whose explanation is as follows. We showed in section V that the function $\Lambda \circ \tau$ (introduced in section IV) is a suitable extension to convex subsets of the function Ω (look at Definition IV.1). We also introduced the physical-informational notion of CSS, an informational invariant convex subset, i.e., a set whose information can be recovered using the sets of its corresponding reduced states. In this sense, *they are informational invariants*. As shown in section V, *they are a suitable generalization of the notion of product state to all convex subsets of \mathcal{C}* .

Thus, as happens in the pure state case, we have developed a generalization which asserts that an arbitrary state is separable if and only if it is an element of an informational invariant that we have called CSS. Our math-constructions and entanglement criteria (linked to the SM measure) highlight

the non-trivial result that the structure found for the pure states case can be properly generalized to arbitrary states, a clear physical simplification.

But the analogy/generalization does not stop here. We can develop still a new analogy/generalization, not contained in the precedent sections. It is well known that another equivalent condition for separability of pure states may be given using von Neuman's entropy, which reads: $\rho = |\psi\rangle\langle\psi|$ is separable if and only if the von Neuman's entropy of its reduced states attains its minimum possible value (zero). In mathematical terms

$$|\psi\rangle\langle\psi| \in \mathcal{S}(\mathcal{H}) \Leftrightarrow S_{vN}(\rho^A) = 0 \\ \text{and } S_{vN}(\rho^B) = 0, \quad (48)$$

where ρ^A and ρ^B are the reduced states of $|\psi\rangle\langle\psi|$ and $S_{vN}(\cdot)$ is the well known von Neuman's entropy functional, defined by

$$S_{vN} = -\text{tr}(\rho \ln(\rho)). \quad (49)$$

Can we concoct something similar for mixed states? Caratheodory's theorem (for finite dimensions) grants that any separable state admits a finite convex decomposition in terms of pure product states. In mathematical terms, this means that there exists pure states $|\varphi_i\rangle\langle\varphi_i| \in \mathcal{C}_1$, $|\phi_i\rangle\langle\phi_i| \in \mathcal{C}_2$ and a finite collection of convex coefficients λ_i such that

$$\rho \in \mathcal{S}(\mathcal{H}) \Leftrightarrow \sum_i \lambda_i (|\varphi_i\rangle\langle\varphi_i|) \otimes (|\phi_i\rangle\langle\phi_i|). \quad (50)$$

It is easy to show that this decomposition combined with our separability criteria VI.1 (look at the demonstration of it) implies that there exists a polytope, call it P_{pure} , whose vertices are just products of pure states. This implies that if we now compute the infimum of the von Neuman entropy evaluated on the elements of P_{pure} we will obtain its minimum value, because as it is well known, von Neuman entropy attains its minimum value for such states. In other words,

$$\inf\{S_{vN}(\rho) \mid \rho \in P_{pure}\} = \min\{S_{vN}(\rho) \mid \rho \in P_{pure}\} = 0. \quad (51)$$

Thus, the analogy advanced in this section is more

than a simple coincidence or mathematical artifice,

because in accord with Eq. (48), we now have that for *any state (pure or mixed)*,

$$\rho \in \mathcal{S}(\mathcal{H}) \Leftrightarrow \exists P_{\text{pure}}, \text{ such that } \min\{S_{vN}(\rho) \mid \rho \in P_{\text{pure}}\} = 0, \quad (52)$$

where P_{pure} represents a polytope whose vertices are products of pure states. Thus, we can sum up some of the results of this article by just using the following words:

Proposition VI.1. *ρ is a separable state \Leftrightarrow it belongs to a CSS (i.e., a convex subset which generalizes product states and is invariant under the function defined by equation (IV.1)) \Leftrightarrow it belongs to a CSS on which the von Neuman's entropy reaches its minimum value.*

The analogy with the pure case is not only clear and suggestive. It may also provide some geometric flavor to the separability problem. It is indeed a generalization which includes the pure case as a special one. Interestingly enough, as shown in section IV, it is strongly linked to the $S-M$ measure.

B. Final conclusions

We have advanced here an abstract criterium of separability and showed that it is closely connected to the extant entanglement measures. We ascertained also that the function $\Lambda \circ \tau$ is a generalization of the map $\rho \mapsto \rho^A \otimes \rho^B$ to convex subsets of \mathcal{C} . Indeed, we showed that $\Lambda \circ \tau$ generalizes to convex sets properties of invariant product states of the map $\rho^A \otimes \rho^B$.

Denoting by “CSS” the invariant subsets of \mathcal{C} , a procedure was delineated that generalizes product states to more general convex sets. This could be useful for the study of new separability criteria based on more general convex subsets of \mathcal{C} and disposes of the obligation of concentrating attention just on points (density matrixes). By itself, the criterium VI.1 also sheds some light into aspects of the geometric properties of separable states.

Appendix A: Notations for basic math concepts used in the text

1. A function is surjective (onto) if every possible image is mapped to by at least one argument. In other words, every element in the codomain has non-empty preimage. Equivalently, a function is surjective if its image is equal to its codomain. A surjective function

is a surjection.

2. Let S be a vector space over the real numbers, or, more generally, some ordered field. A set C in S is said to be convex if, for all x and y in C and all t in the interval $[0, 1]$, the point $(1-t)x + ty$ is in C . That is, every point on the line segment connecting x and y belongs to C . This entails that any convex set in a real or complex topological vector space is path-connected.
3. Every subset Q of a vector space is contained within a smallest convex set (called the convex hull of Q), namely the intersection of all convex sets containing Q ,
4. Suppose that K is a field (for example, the real numbers) and V is a vector space over K . If v_1, \dots, v_n are vectors and a_1, \dots, a_n are scalars, then the linear combination of those vectors with those scalars as coefficients is, of course, $\sum_{i=1}^n a_i v_i$. By restricting the coefficients used in linear combinations, one can define the related concepts of affine combination, conical combination, and convex combination, together with the associated notions of sets closed under these operations. If $\sum_{i=1}^n a_i = 1$, we have an affine combination, its span being an affine subspace while the model space is an hyperplane. If $a_i \geq 0$, we have instead a conical combination, a convex cone and a quadrant, respectively. Finally, if $a_i \geq 0$ plus $\sum_{i=1}^n a_i = 1$ we have now a convex combination, a convex set and a simplex, respectively.

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